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DFT Study of the Structure, Spectroscopy and Properties of Biomolecules

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Message from the Guest Editor

DFT methods provide invaluable information, complementary to experimental data, on molecular systems and processes and, therefore, they represent very powerful tools for the interpretation and understanding of the experimental results. These methods, combined with quantum mechanics (QM), Molecular mechanics (MM), molecular docking and others, are very useful for the fundamental understanding of structure–activity relationships in biomolecules and also for applications in drug design and biotechnology.<false,>This Special Issue tries to introduce new interesting developments in the field of the molecular structure, vibrational spectroscopy and properties of biomolecules, especially those with chemical, pharmaceutical or biological interest. DFT applications to biomolecules, including molecular optimizations, structure predictions, inter-molecular interactions, spectroscopic calculations, as well as theoretical developments and experiments are welcome.

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Message from the Editor-in-Chief

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